

Breakdown of the initial value formulation of scalar-tensor gravity and its physical meaning

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We revisit singularities of two distinct kinds in the Cauchy problem of general scalar-tensor theories of gravity (previously discussed in the literature), and of metric and Palatini $f(R)$ gravity, in both their Jordan and Einstein frame representations. Examples and toy models are used to shed light onto the problem and it is shown that, contrary to common lore, the two conformal frames are equivalent with respect to the initial value problem.

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I. INTRODUCTION

The 1998 discovery of the acceleration of the cosmic expansion, obtained by studying type Ia supernovae [1], spurred an enormous amount of activity on dark energy models, mostly based on cosmological scalar fields. Certain models are set in the context of scalar-tensor gravity instead of Einstein's theory, and are dubbed "extended quintessence" [2]. Moreover, as an alternative to postulating a mysterious form of dark energy, various authors ([3, 4], see [5] for a review) have considered the possibility that the acceleration of the universe is caused instead by a modification of gravity at large scales: the Einstein-Hilbert action

$$S_{EH} = \frac{1}{2\kappa} \int d^4x \sqrt{-g} R + S^{(m)}[g_{ab}, \psi] \quad (1)$$

is generalized to

$$S = \frac{1}{2\kappa} \int d^4x \sqrt{-g} f(R) + S^{(m)}[g_{ab}, \psi], \quad (2)$$

where $f(R)$ is an arbitrary, twice differentiable, function of R . Here $\kappa \equiv 8\pi G$, G is Newton's constant (that will be unity, together with the speed of light, in the geometrized units employed), R is the Ricci curvature, $S^{(m)} = \int d^4x \sqrt{-g} \mathcal{L}^{(m)}[g_{ab}, \psi]$ is the matter part of the action, ψ collectively denotes the matter fields, and we follow the notations of [6].

If the action (2) is varied with respect to the metric g_{ab} , one obtains the *metric formalism* with fourth order field equations [3, 4]; if the metric and the connection Γ_{bc}^a are considered as independent variables (*i.e.*, the connection is not the metric connection of g_{ab}), but the matter part of the action $S^{(m)}$ does not depend explicitly on Γ , one obtains the *Palatini formalism* with second order field equations [7]. If, instead, $S^{(m)}$ depends on Γ , one obtains *metric-affine* gravity [8].

It has been shown [9] that metric $f(R)$ gravity is dynamically equivalent to a Brans-Dicke (BD) theory with BD parameter $\omega_0 = 0$, while Palatini $f(R)$ gravity is equivalent to an $\omega_0 = -3/2$ BD theory. The general form of the scalar-tensor action, of which BD theory [10, 11] is the prototype, is [12]

$$S_{ST} = \int d^4x \sqrt{-g} \left[\frac{f(\phi)R}{2} - \frac{\omega(\phi)}{2} \nabla^c \phi \nabla_c \phi - V(\phi) \right] + S^{(m)}[g_{ab}, \psi], \quad (3)$$

where ϕ is the BD-like scalar field and $f(\phi) > 0$ is required in order for the effective gravitational coupling to be positive and the graviton to carry positive kinetic energy and not being a ghost. $V(\phi)$ is the scalar field potential, while $f(\phi)$ and $\omega(\phi)$ are two (*a priori* arbitrary) coupling functions. BD theory is recovered as the special case $f(\phi) = \phi$ and $\omega(\phi) = \omega_0/\phi$, with $\omega_0 = \text{const}$. The field equations derived from the action (3) are

$$f(\phi) \left(R_{ab} - \frac{1}{2} g_{ab} R \right) = \omega(\phi) \left(\nabla_a \phi \nabla_b \phi - \frac{1}{2} g_{ab} \nabla^c \phi \nabla_c \phi \right) - V g_{ab} + \nabla_a \nabla_b f - g_{ab} \square f + T_{ab}^{(m)}, \quad (4)$$

$$\left[\omega + \frac{3(f')^2}{2f} \right] \square \phi + \left(\frac{\omega'}{2} + \frac{3f'f''}{2f} + \frac{\omega f'}{2f} \right) \nabla_c \phi \nabla^c \phi = \frac{f'}{2f} T + 2V' - \frac{2Vf'}{f}, \quad (5)$$

where a prime denotes differentiation with respect to ϕ , $\square \equiv g^{ab} \nabla_a \nabla_b$, and $T_{ab} = \frac{-2}{\sqrt{-g}} \frac{\delta S^{(m)}}{\delta g^{ab}}$.

The original motivation for BD theory was the implementation in relativistic gravity of the Mach principle, which is not fully embodied in general relativity, by promoting Newton's constant to the role of a dynamical field determined by the environment [10, 11]. Later on, it was discovered that string theories and supergravity contain BD-like scalars: in fact, the low energy limit of the bosonic string theory (which, although unphysical because it does not contain fermions and is not supersymmetric, was one of the early string theories) is indeed an $\omega_0 = -1$ BD theory [13]. Moreover, BD theory can be derived from higher-dimensional Kaluza-Klein theory, higher dimensionality being an essential feature of all modern high energy theories. A p -brane model in D dimensions leads, after compactification, to a BD theory with parameter [14]

$$\omega_0 = -\frac{(D-1)(p-1) - (p+1)^2}{(D-2)(p-1) - (p+1)^2}. \quad (6)$$

These properties have renewed the interest in BD and scalar-tensor gravity since the 1980s, following the rise of string theory. However, the more recent surge of interest in scalar-tensor gravity that we are witnessing is motivated by cosmology and is linked to attempts to explain the present cosmic acceleration (see [15, 16] for reviews of scalar-tensor gravity in the cosmology of the early and present universe).

Motivated by the past and recent interest and also by developments in numerical relativity, the initial value problem of scalar-tensor gravity was studied by Salgado [17] who, using a first order hyperbolicity analysis, showed that the Cauchy problem is well-formulated for theories of the form

$$S = \int d^4x \sqrt{-g} \left[\frac{f(\phi)R}{2} - \frac{1}{2} \nabla^c \phi \nabla_c \phi - V(\phi) \right] + S^{(m)}[g_{ab}, \psi] \quad (7)$$

when $S^{(m)}$ is “reasonable” [51] and is well-posed in vacuo. It was then straightforward to generalize this work to BD theories with constant BD parameter $\omega_0 \neq 1$ which, in turn, was used to show that the Cauchy problem of metric $f(R)$ gravity (equivalent to an $\omega_0 = 0$ BD theory) is well-formulated and well-posed in vacuo, while the Cauchy problem for Palatini $f(R)$ gravity (equivalent to an $\omega_0 = -3/2$ BD theory) is not well-formulated, nor well-posed [19]. A second paper by Salgado and co-workers using a second order hyperbolicity analysis [20] showed the well-posedness of $\omega = 1$ theories, and the extension to $\omega = \text{const.}$ theories (with the exception of $\omega = -3/2$) is straightforward because the principal part of the field equations does not depend on ω .

In retrospect, it is easy to see why the $\omega_0 = -3/2$ BD theory does not admit a well-posed initial value formula-

tion: the field equation for the BD scalar is

$$\left(\omega_0 + \frac{3}{2} \right) \square \phi + \frac{\omega_0}{2\phi} \nabla^c \phi \nabla_c \phi = \frac{T}{2\phi} + V' - \frac{2V}{\phi}, \quad (8)$$

and reduces to a first order constraint when $\omega_0 \rightarrow -3/2$. Technically, this fact prevents the substitution of $\square \phi$ back into the equations for the other dynamical variables in order to eliminate second derivatives of ϕ and spoils the reduction to a first-order system (see [19] for details). In practice, the second order dynamical equation for the variable ϕ is lost when $\omega_0 = -3/2$, ϕ then plays the role of a non-dynamical auxiliary field and can be assigned arbitrarily *a priori*. Uniqueness of the solutions is then lost, as infinitely many prescriptions for ϕ correspond to the same set of initial data.

The present paper serves various purposes. First (Sec. II), we revisit the Cauchy problem for BD theories and, in particular, for the equivalent of Palatini $f(R)$ gravity by using a completely independent approach based on the transformation to the Einstein conformal frame. This approach was deliberately avoided in previous papers [17, 19, 20]. While interesting in itself as an independent check of previous results, this approach has the additional merit of fully establishing the physical equivalence between Jordan and Einstein frames at the classical level. These conformal frames have been shown to be equivalent in various other respects, and it would only make sense that their equivalence extend to the Cauchy problem. However, there are explicit statements in the literature, and much unwritten folklore, pointing to the contrary. We show here that the two frames are indeed equivalent, which removes previous doubts and fully establishes equivalence at the classical level; however, this does not guarantee physical equivalence at the quantum level [21, 22].

The main purpose of this paper, however, consists of the study of the Cauchy problem for scalar-tensor theories of the general form (3) and of two distinct types of singularities that may appear in their field equations. These theories were not covered explicitly in previous literature, although the extension of the results of [17, 20] to include them is relatively straightforward. In addition, it is handy to consider the general form (3) of the theory in order to specialize the results to any scalar-tensor theory simply by prescribing specific forms of the coupling functions $f(\phi)$ and $\omega(\phi)$ and of the potential $V(\phi)$. We approach the problem in both the Jordan frame (Sec. III) and the Einstein frame (Sec. IV) obtaining, of course, the same results.

In general scalar-tensor theories, there are two kinds of singularities to deal with: those at which $f(\phi) = 0$, and a second kind identified by $f_1(\phi) \equiv \omega(\phi) + \frac{3(f'(\phi))^2}{2f(\phi)} = 0$, which generalizes the $\omega_0 = -3/2$ pathology encountered in BD theory and in Palatini $f(R)$ gravity. Singularities of the first kind should normally be excluded by requiring

that $f(\phi) > 0$ for all values of ϕ , and this requirement is sometimes made explicit in the general formalism (*e.g.*, [23]); nevertheless, works incorporating these singularities recur often in the literature, especially in cosmology.

At the singularities of the second kind $f_1 = 0$ (which have been known for a long time in particular incarnations of scalar-tensor gravity [24, 25, 26]), a phenomenology similar to that of Palatini $f(R)$ gravity spoils the Cauchy problem for special forms of the coupling function $\omega(\phi)$, or for critical field values. While the scalar field is allowed to pass through these “singularities” in an isotropic Friedmann-Lemaître-Robertson-Walker (FLRW) universe [24, 25, 26], the points where $f_1(\phi) = 0$ are known to give rise to curvature and shear singularities in the anisotropic case. These singularities were discovered in the special case of nonminimally coupled scalar field cosmology (corresponding to $f(\phi) = \frac{1}{\kappa} - \xi\phi^2$ and $\omega = 1$) in the early universe [24, 25, 27, 28] and also in black hole perturbations [29]. They also appear in the search for exact wormhole solutions with nonminimally coupled scalar fields [30]. Singularities of both kinds were discussed in a more general context in [31, 32]. After clarifying and further generalizing this situation from the point of view of the initial value formulation in Sec. III, in Sec. IV we revisit this subject in the Einstein frame, exposing a situation analogous to $\omega_0 = -3/2$ BD theory (this is not merely an analogy, since the latter is a special case of the former). Finally, in Sec. V, we study nonminimally coupled scalar field theory as an example, recovering certain known properties and placing them in a general context. Sec. VI and VII contain illustrative toy models and the conclusions, respectively.

II. EINSTEIN FRAME DESCRIPTION OF BRANS-DICKE AND PALATINI $f(R)$ GRAVITY

In this section we recall the definition of Einstein conformal frame and show explicitly the non-dynamical role of the scalar field in the Einstein frame representation of the scalar-tensor version of Palatini $f(R)$ gravity. This is necessary as a first step to understand the more involved situation that we will be facing in later sections with general scalar-tensor theories of the form (3).

The conformal transformation

$$g_{ab} \rightarrow \tilde{g}_{ab} = \Omega^2 g_{ab}, \quad \Omega = \sqrt{\tilde{\phi}} \quad (9)$$

and the scalar field redefinition $\phi \rightarrow \tilde{\phi}$ with

$$d\tilde{\phi} = \sqrt{\frac{|2\omega_0 + 3|}{2\kappa}} \frac{d\phi}{\phi} \quad (10)$$

map the Jordan frame action of BD theory

$$S_{BD} = \int d^4x \sqrt{-g} \left[\frac{\phi R}{2} - \frac{\omega_0}{2\phi} \nabla^c \phi \nabla_c \phi - V(\phi) + \mathcal{L}^{(m)} \right] \quad (11)$$

into its Einstein frame representation

$$S_{BD} = \int d^4x \sqrt{-\tilde{g}} \left[\frac{\tilde{R}}{2\kappa} - \frac{1}{2} \tilde{g}^{ab} \tilde{\nabla}_a \tilde{\phi} \tilde{\nabla}_b \tilde{\phi} - U(\tilde{\phi}) + \frac{\mathcal{L}^{(m)} [\Omega^{-1} \tilde{g}_{ab}, \psi]}{\phi^2} \right], \quad (12)$$

where

$$U(\tilde{\phi}) = \frac{V(\phi(\tilde{\phi}))}{\phi^2(\tilde{\phi})} \quad (13)$$

and a tilde denotes rescaled (Einstein frame) quantities. The scalar field redefinition (10) breaks down when $\omega_0 = -3/2$ and the scalar field $\tilde{\phi}$ then remains undefined. However, eq. (9) still holds and one can write the Einstein frame version of the BD equivalent of Palatini $f(R)$ gravity as [5]

$$S_{Palatini} = \frac{1}{2\kappa} \int d^4x \sqrt{-\tilde{g}} \left[\tilde{R} - \frac{V(\phi)}{\phi^2} \right] + S^{(m)} [\phi^{-1} \tilde{g}_{ab}, \psi] \quad (14)$$

using the variables (\tilde{g}_{ab}, ϕ) . In this action, the scalar field ϕ does not play any dynamical role: it only acts as a factor rescaling the metric in $S^{(m)}$ but it has no dynamics, does not couple to \tilde{R} , and no kinetic energy of ϕ appears in (14). ϕ can be assigned arbitrarily in infinitely many ways not governed by the usual second order differential equation and, therefore, uniqueness of the solutions is lost. On the contrary, for any value of the BD parameter $\omega_0 \neq -3/2$ (in particular for the $\omega_0 = 0$ equivalent of metric $f(R)$ gravity), the action is reduced to (12), which describes a scalar field $\tilde{\phi}$ coupling minimally to the curvature and nonminimally to matter. In vacuo ($\mathcal{L}^{(m)} = 0$), this coupling to matter disappears and we are left with the action of Einstein gravity plus a minimally coupled scalar field with canonical kinetic energy: it is well-known that this system has a well-posed initial value formulation [6, 18]. The non-vacuum case is considered later in Sec. V as a special case of more general scalar-tensor theories.

III. THE CAUCHY PROBLEM FOR GENERAL SCALAR-TENSOR THEORIES IN THE JORDAN FRAME

Let us now restrict ourselves to the Jordan frame and consider general scalar-tensor theories described by the action (3). These can be reduced to the action

$$S = \int d^4x \sqrt{-g} \left[\frac{\Phi R}{2} - \frac{\omega^*(\Phi)}{2} \nabla^c \Phi \nabla_c \Phi - U(\Phi) \right] + S^{(m)} \quad (15)$$

containing a single coupling function $\omega^*(\Phi)$ by setting $\Phi \equiv f(\phi)$, $\omega^*(\Phi) = \omega(\phi(\Phi))$, and $U(\Phi) = V(\phi(\Phi))$. The actions (3) and (15) are equivalent if $f(\phi)$ is invertible with regular inverse f^{-1} , but this does not happen if $f'(\phi)$ vanishes somewhere.

It is also possible to recast BD theory as one in which the kinetic term of the scalar field is canonical, *i.e.*, with $\omega = 1$. Beginning with the action (15) and setting

$$\Phi = F(\varphi) , \quad (16)$$

where the function $F(\varphi)$ is defined by the equation

$$\omega^*(\Phi) = \frac{F(\varphi)}{2 \left(\frac{dF}{d\varphi} \right)^2} , \quad (17)$$

(15) can be rewritten as

$$S = \int d^4x \sqrt{-g} \left[\frac{F(\varphi)R}{2} - \frac{1}{2} \nabla^c \varphi \nabla_c \varphi - W(\varphi) \right] + S^{(m)}[g_{ab}, \psi] , \quad (18)$$

where $W(\varphi) = V[F(\varphi)]$. This alternative form of the BD action can not be obtained when $F(\varphi)$ does not admit a regular inverse F^{-1} (*e.g.*, when $dF/d\varphi = 0$). This is the case, for example, when $F(\varphi)$ is represented by a series of even powers of φ [33, 34]. Note that (18) is the form of the action considered in the studies of the Cauchy problem [17, 20]. In what follows, to achieve full generality, we discuss the action (3) with two coupling functions. Moreover, there are two types of “singularities” to consider: we introduce them here and we will refer to them for the rest of this paper. In addition, one must distinguish between two very different situations: that in which these “singularities” occur in an entire four-dimensional domain of spacetime, and that in which they occur only on hypersurfaces. Moreover, we will approach all of the above from the two viewpoints of Jordan frame and Einstein frame.

Singularities of the first kind

The first type of singularities is identified by $f(\phi_*) = 0$ and occurs for critical values ϕ_* of the scalar field (if solutions of this equation exist). This equation may be satisfied in an entire four-dimensional spacetime region, or on a hypersurface. At a first glance, the former case seems rather trivial: in fact, naively, the effective gravitational coupling read off the action (26) is $G_{eff} = 1/f(\phi)$. However, a more careful analysis of the effective gravitational coupling in a Cavendish experiment, which is the only one directly accessible to local experiments, yields [35]

$$G_{eff}(\phi) = \frac{2\omega f + (2df/d\phi)^2}{8\pi f \left[2\omega f + 3(df/d\phi)^2 \right]} . \quad (19)$$

This expression can also be obtained from the study of cosmological perturbations [36]. The first type of singularities $f(\phi_*) = 0$ corresponds to diverging effective coupling $G_{eff}(\phi)$ and separates regions in which G_{eff} has opposite signs describing attractive or repulsive gravity, respectively. Stated this way, it may seem nonsensical to consider such values ϕ_* of the scalar. For example, it looks plain silly to consider, in BD theory, a spacetime region in which $\phi = 0$, which makes the term $\phi R/2$ disappear from the BD action and corresponds to infinite strength of gravity. Nevertheless, there are examples in which exact (and non-unique) solutions of the field equations have been found with ϕ constant and precisely equal to ϕ_* in a region, or in the entire spacetime manifold (see [26, 37, 38] for examples in cosmology and [30] for wormhole solutions). Are these to be discarded *a priori*? Perhaps not, because what is clearly unphysical are regions in which $G_{eff} < 0$ and the graviton is a ghost. Although rather pathological, regions in which G_{eff} is divergent may still be interesting in exotic situations when the birth of the universe or the interior of a wormhole are considered. Furthermore, these regions may still be relevant from the mathematical point of view if one is interested in finding exact solutions that, as simplified toy models, exhibit particular properties of scalar-tensor gravity.

Let us come now to the more interesting situation in which $f(\phi) = 0$ *on an hypersurface*. This situation seems more reasonable, however such hypersurfaces separate regions of attractive from regions of repulsive gravity; in the latter, the graviton carries negative kinetic energy, a physically unacceptable property [23, 39]. This fact seems to be forgotten in scalar-tensor theories more general than BD theory and with more freedom in the form of the functions $f(\phi)$ and $\omega(\phi)$. Papers in which G_{eff} is negative or infinite have appeared surprisingly often over the past thirty years [26, 27, 28, 40, 41, 42, 43]; sometimes, such critical hypersurfaces ϕ_* are approached asymptotically [52].

Let us proceed, for the moment, by adopting a purely mathematical point of view in the consideration of the Cauchy problem. When $f(\phi) = 0$, eq. (4) for the metric tensor degenerates. At these spacetime points the trace of eq. (4) becomes

$$3\Box\phi + (\omega + 3f'') \nabla^c \phi \nabla_c \phi + 4V - T = 0 . \quad (20)$$

Substitution of the value of $\Box\phi$ obtained from this equation into the second field equation (5) yields

$$R = \frac{2}{f'} \left\{ \left[\frac{\omega'}{2} - \frac{\omega}{3f'} (\omega + 3f'') \right] \nabla^c \phi \nabla_c \phi + \frac{\omega}{3f'} (T - 4V) - 2V' \right\} . \quad (21)$$

Knowledge of the values of ϕ and of its gradient $\nabla_c \phi$ on the hypersurface $f = 0$ determines the Ricci curva-

ture. However, the equation for R_{ab} disappears there, which means that all metrics with the same value of R satisfy the (degenerate) field equations on this hypersurface: uniqueness of the solutions is lost and this surface is a Cauchy horizon. The initial value problem breaks down at these critical points. Therefore, even if we decide to allow the unphysical region $G_{eff} < 0$ by attempting to propagate initial data given in a $G_{eff} > 0$ region, we encounter a hypersurface on which $G_{eff} \rightarrow \infty$ which acts as a barrier and the initial value formulation ceases to be well-posed.

Singularities of the second kind

Let us introduce now a second type of critical values of the scalar field that have previously been associated to physical (curvature) singularities and that also correspond to a breakdown of the initial value problem. Following the lesson of $\omega = -3/2$ theory [19], one notices that $\square\phi$ disappears from the field equation (5) when

$$f_1(\phi) \equiv \omega(\phi) + \frac{3(f'(\phi))^2}{2f(\phi)} = 0. \quad (22)$$

Again, one has to distinguish two cases: a) eq. (22) is satisfied in a four-dimensional spacetime region, and b) it is satisfied on a hypersurface. The former corresponds to regarding eq. (22) as specifying a particular form of the coupling function $\omega(\phi)$ (given $f(\phi)$), while the latter corresponds to seeing eq. (22) as a transcendental (or algebraic, depending on the forms of the functions ω and f) equation that may admit as roots special critical values ϕ_c of the scalar ϕ [53].

Let us consider case a) first: this is completely analogous to the case of $\omega = -3/2$ BD theory which eq. (22) generalizes. When $f_1(\phi)$ vanishes identically for all values of ϕ in a four-dimensional spacetime domain, the dynamics of the scalar ϕ are lost together with $\square\phi$ and with the second order of the partial differential equation for ϕ . The exception consists of situations in which the scalar satisfies $\square\phi = 0$, in which case there may be non-trivial dynamics for ϕ , but this quantity disappears spontaneously from the field equations for the other variables. This situation includes general relativity with $\phi = \text{const.}$ (for which the initial value problem is well-posed [6] and the previous discussion obviously does not apply), and harmonic ϕ -waves.

Situation a) is, of course, the only possibility when ω represents a constant parameter instead of a function, as in BD theory. The general scalar-tensor theory is richer and allows one to contemplate the possibility b) that eq. (22) is satisfied on a hypersurface. It is interesting that, in the absence of matter, invariants of the Riemann tensor diverge at this hypersurface for anisotropic metrics, while no such divergence occurs in isotropic FLRW

spaces [25, 31]. Mathematically speaking, if $f(\phi) \neq 0$ and $f_1(\phi)$ is a continuous function, a hypersurface where $f_1(\phi) = 0$ separates two regions corresponding to opposite signs of f_1 (unless the form of f_1 is pathologically fine-tuned): in each of these, the Cauchy problem may be well-posed but when one tries to propagate initial data through such a hypersurface, $\square\phi$ given by

$$\square\phi = \left\{ -\left(\frac{\omega'}{2} + \frac{3f'f''}{2f} + \frac{\omega f'}{2f}\right) \nabla_c \phi \nabla^c \phi + \frac{f'T}{2f} + 2V' - \frac{2Vf'}{f} \right\} \left[\omega + \frac{3(f')^2}{2f} \right]^{-1} \quad (23)$$

diverges. We have, therefore, a Cauchy horizon that is not hidden inside an apparent horizon, as in black holes, and where the theory crashes. The two regions separated by the hypersurface $f_1(\phi) = 0$ are, again, disconnected by a singularity in the gravitational coupling $G_{eff}(\phi)$.

To summarize this section: when the coupling functions $f(\phi)$ and $\omega(\phi)$ are such that $f(\phi) = 0$ or $f_1(\phi) = 0$, the initial value formulation breaks down and either the theory is unphysical because ϕ becomes a non-dynamical auxiliary field, or the hypersurface $f_1(\phi) = 0$ is a Cauchy horizon. In the first case, the problems found for Palatini $f(R)$ gravity in [45] re-surface. The situation in which eq. (22) is identically satisfied is the generalization to arbitrary scalar-tensor theories of the situation already seen in $\omega = -3/2$ BD theory and in Palatini $f(R)$ gravity. The trace equation (20) allows one to replace the trace T with an expression containing second derivatives of ϕ . Then, the metric depends on derivatives of the scalar field of order higher than second and discontinuities, or irregularities, are not smoothed out by an integral of matter fields giving the metric g_{ab} (for example, as in the usual Green function integral in the weak-field limit), but they cause step-function discontinuities in the metric derivatives and curvature singularities where the same matter distribution in Einstein's theory would generate a perfectly regular geometry.

IV. GENERAL SCALAR-TENSOR THEORIES AND THE CAUCHY PROBLEM IN THE EINSTEIN FRAME

We now examine the initial value problem of general scalar-tensor gravity in the Einstein frame. The conformal transformation

$$g_{ab} \rightarrow \tilde{g}_{ab} = \Omega^2 g_{ab}, \quad \Omega = \sqrt{f(\phi)} \quad (24)$$

and the scalar field redefinition

$$\tilde{\phi} = \int \sqrt{|2\omega f + 3(f')^2|} \frac{d\phi}{f(\phi)} \quad (25)$$

bring the Jordan frame action

$$S = \int d^4x \sqrt{-g} \left[\frac{f(\phi)R}{2} - \frac{\omega(\phi)}{2} \nabla^c \phi \nabla_c \phi - V(\phi) + \mathcal{L}^{(m)} \right] \quad (26)$$

into its Einstein frame representation

$$S = \int d^4x \sqrt{-\tilde{g}} \left[\frac{\tilde{R}}{2\kappa} - \frac{1}{2} \tilde{g}^{ab} \tilde{\nabla}_a \tilde{\phi} \tilde{\nabla}_b \tilde{\phi} - U(\tilde{\phi}) + \frac{\mathcal{L}^{(m)}}{f^2} \right], \quad (27)$$

where $U(\tilde{\phi}) = V(\phi(\tilde{\phi}))/f^2$ and $f = f(\phi(\tilde{\phi}))$. Again, apart from the now familiar coupling of the “new” scalar $\tilde{\phi}$ to matter described by $\mathcal{L}^{(m)}/f^2$ (with the exception of conformally invariant matter), this action describes general relativity with a canonical scalar field which couples minimally to the curvature but nonminimally to matter. As before, it is clear that the system has a well-posed initial value formulation in vacuo. This conclusion applies where the Einstein frame variables $(\tilde{g}_{ab}, \tilde{\phi})$ are well-defined, *i.e.*, for $f(\phi) \neq 0$ and $f_1(\phi) \neq 0$. It can be shown that the Cauchy problem is well-posed in the presence of matter as well: this was already pointed out in ref. [23], but is checked at the end of this section by extending the first order hyperbolicity analysis of [17].

The exception is when $f_1(\phi) = 0$, in which case the scalar $\tilde{\phi}$ can not be defined using eq. (25). In this case, one can use the variables (\tilde{g}_{ab}, ϕ) instead of $(\tilde{g}_{ab}, \tilde{\phi})$, obtaining the Einstein frame action

$$S_{ST} = \int d^4x \sqrt{-\tilde{g}} \left[\frac{\tilde{R}}{2\kappa} - \frac{V(\phi)}{f^2(\phi)} - \frac{\mathcal{L}^{(m)}}{f^2(\phi)} \right]. \quad (28)$$

Again, there are no dynamics for ϕ and the Cauchy problem is not well-formulated, nor well-posed, in this case due to the loss of uniqueness of the solutions. Moreover, this result holds in both the Jordan and the Einstein frames, which then become physically equivalent in this respect.

The breakdown of the scalar field redefinition (25) is accompanied by other signals that something is going wrong with the physics when $f_1(\phi) = 0$. The effective gravitational coupling (19) diverges when $f_1 = 0$ (as a special case, $G_{eff} = \frac{2(2\omega_0+2)}{(2\omega_0+3)\phi}$ diverges as $\omega_0 \rightarrow -3/2$ in BD theory). Moreover, it changes sign when ϕ crosses a critical value ϕ_* or ϕ_c . These critical values are attained by the scalar field in certain early universe inflationary scenarios with nonminimally coupled scalar fields, corresponding to $f(\phi) = \frac{1}{\kappa} - \xi\phi^2$ and $\omega = 1$ (ξ being a dimensionless coupling constant) when $0 < \xi < 1/6$ [24, 25, 26, 28]. The same phenomenon in more general scalar-tensor theories is considered in [31, 32].

The authors of [31] find that, in Bianchi cosmologies, the regions of the phase space at which $f_1(\phi) = 0$ correspond to geometric singularities with divergent Kretschmann scalar $R_{abcd}R^{abcd}$. The $f_1 = 0$ singularity is dynamically forbidden in a closed or critically open

FLRW universe under the assumptions $\rho \geq 0, V(\phi) \geq 0$, and $\omega \geq 1$ [32].

The lesson of [25, 28, 31] is that, if there is even a small anisotropy, the change from attractive to repulsive gravity at $f_1 = 0$ can only occur through a shear or curvature singularity which stops the evolution of the geometry: nature’s message seems to be that gravity can not spontaneously become repulsive in the absence of exotic matter violating the energy conditions (it is the purely gravitational sector of the theory that we are studying here).

Note that in the theories considered by [31, 32], which have $\omega \equiv 1$, the singularity $f_1 = 0$ is automatically removed by requiring that $f(\phi) > 0$ (*i.e.*, that the graviton is not a ghost); however, this is no longer true when theories with ω not identically equal to unity are considered and critical values ϕ_c of the second kind can still occur even when $f(\phi) > 0 \forall \phi$ — but this necessarily requires $\omega < 0$.

Let us now extend the first order hyperbolicity analysis of [17] to Einstein frame scalar-tensor gravity. We follow closely, and adopt the notations of, [17, 19] in order to facilitate comparison, setting $\kappa = 1$. The Einstein frame field equations are

$$\begin{aligned} \tilde{G}_{ab} &= \tilde{\nabla}_a \tilde{\phi} \tilde{\nabla}_b \tilde{\phi} - \frac{1}{2} \tilde{g}_{ab} \tilde{\nabla}^c \tilde{\phi} \tilde{\nabla}_c \tilde{\phi} - U(\tilde{\phi}) \tilde{g}_{ab} \\ &+ \frac{T_{ab}^{(m)}}{f^2(\phi(\tilde{\phi}))} \equiv \tilde{T}_{ab}[\tilde{\phi}] + \tilde{T}_{ab}^{(m)} \equiv \tilde{T}_{ab}, \end{aligned} \quad (29)$$

$$\tilde{\square} \tilde{\phi} - \frac{dU(\tilde{\phi})}{d\tilde{\phi}} = 0. \quad (30)$$

Because $T_{ab}[\tilde{\phi}]$ does not contain second derivatives of $\tilde{\phi}$, it is possible to give a first order formulation as in general relativity. The nonminimal coupling factor $1/f^2(\phi(\tilde{\phi}))$ multiplying $T_{ab}^{(m)}$ on the right hand side of eq. (29) does not generate derivatives of $\tilde{\phi}$ and therefore is immaterial.

The 3 + 1 ADM formulation of the theory defines the usual lapse, shift, extrinsic curvature, and gradients of ϕ [6, 17]. Assuming the existence of a time function t such that the spacetime (M, \tilde{g}_{ab}) is foliated by a family of hypersurfaces Σ_t of constant t with unit timelike normal \tilde{n}^a , the 3-metric is defined by $\tilde{h}_{ab} = \tilde{g}_{ab} + \tilde{n}_a \tilde{n}_b$ and \tilde{h}_c^a is the projection operator on Σ_t . The relations $\tilde{n}^a \tilde{n}_a = -1$, $\tilde{h}_{ab} \tilde{n}^b = \tilde{h}_{ab} \tilde{n}^a = 0$, and $\tilde{h}_a^b \tilde{h}_{bc} = \tilde{h}_{ac}$ are satisfied. Further introducing the lapse \tilde{N} , shift vector \tilde{N}^a , and spatial metric \tilde{h}_{ij} , the metric is written as

$$d\tilde{s}^2 = -(\tilde{N}^2 - \tilde{N}^i \tilde{N}_i) dt^2 - 2\tilde{N}_i dt dx^i + \tilde{h}_{ij} dx^i dx^j \quad (31)$$

($i, j = 1, 2, 3$), with $\tilde{N} > 0$, $\tilde{n}_a = -\tilde{N} \tilde{\nabla}_a t$ and

$$\tilde{N}^a = -\tilde{h}_b^a t^b, \quad (32)$$

where the time flow vector \tilde{t}^a satisfies $\tilde{t}^a \tilde{\nabla}_a t = 1$ and

$$\tilde{t}^a = -\tilde{N}^a + \tilde{N} \tilde{n}^a \quad (33)$$

so that $\tilde{N} = -\tilde{n}_a \tilde{t}^a$ and $\tilde{N}^a \tilde{n}_a = 0$. The extrinsic curvature of Σ_t is

$$\tilde{K}_{ab} = -\tilde{h}_a^c \tilde{h}_b^d \tilde{\nabla}_c \tilde{n}_d. \quad (34)$$

The 3D covariant derivative of \tilde{h}_{ab} on Σ_t is defined as

$$\tilde{D}_i^{(3)} T^{a_1 \dots b_1 \dots} = \tilde{h}_{c_1}^{a_1} \dots \tilde{h}_{b_1}^{d_1} \dots \tilde{h}_i^f \tilde{\nabla}_f^{(3)} T^{c_1 \dots d_1 \dots} \quad (35)$$

for any 3-tensor $^{(3)}T^{a_1 \dots b_1 \dots}$, with $\tilde{D}_i \tilde{h}_{ab} = 0$. The spatial gradient of the scalar field and its momentum are

$$\tilde{Q}_a \equiv \tilde{D}_a \tilde{\phi}, \quad (36)$$

and

$$\tilde{\Pi} = \mathcal{L}_{\tilde{n}} \tilde{\phi} = \tilde{n}^c \tilde{\nabla}_c \tilde{\phi}, \quad (37)$$

respectively, and

$$\tilde{K}_{ij} = -\tilde{\nabla}_i \tilde{n}_j = -\frac{1}{2\tilde{N}} \left(\frac{\partial \tilde{h}_{ij}}{\partial t} + \tilde{D}_i \tilde{N}_j + \tilde{D}_j \tilde{N}_i \right), \quad (38)$$

$$\tilde{\Pi} = \frac{1}{\tilde{N}} \left(\partial_t \tilde{\phi} + \tilde{N}^c \tilde{Q}_c \right), \quad (39)$$

$$\partial_t \tilde{Q}_i + \tilde{N}^l \partial_l \tilde{Q}_i + \tilde{Q}_l \partial_i \tilde{N}^l = \tilde{D}_i \left(\tilde{N} \tilde{\Pi} \right). \quad (40)$$

The stress-energy tensor is 3 + 1-decomposed as

$$\tilde{T}_{ab} = \tilde{S}_{ab} + \tilde{J}_a \tilde{n}_b + \tilde{J}_b \tilde{n}_a + \tilde{E} \tilde{n}_a \tilde{n}_b, \quad (41)$$

where

$$\tilde{S}_{ab} \equiv \tilde{h}_a^c \tilde{h}_b^d \tilde{T}_{cd} = \tilde{S}_{ab}[\tilde{\phi}] + \tilde{S}_{ab}^{(m)}, \quad (42)$$

$$\tilde{J}_a \equiv -\tilde{h}_a^c \tilde{T}_{cd} \tilde{n}^d = \tilde{J}_a[\tilde{\phi}] + \tilde{J}_a^{(m)}, \quad (43)$$

$$\tilde{E} \equiv \tilde{n}^a \tilde{n}^b \tilde{T}_{ab} = \tilde{E}[\tilde{\phi}] + \tilde{E}^{(m)}, \quad (44)$$

and $\tilde{T} = \tilde{S} - \tilde{E}$, where \tilde{T} is the trace of \tilde{T}_{ab} and \tilde{S} is the trace of \tilde{S}_{ab} . The Gauss-Codacci equations provide the Einstein equations projected tangentially and orthogonally to Σ_t as the Hamiltonian constraint [6, 17]

$$^{(3)}\tilde{R} + \tilde{K}^2 - \tilde{K}_{ij} \tilde{K}^{ij} = 2\tilde{E}, \quad (45)$$

the vector (or momentum) constraint

$$\tilde{D}_l \tilde{K}^l_i - \tilde{D}_i \tilde{K} = \tilde{J}_i, \quad (46)$$

and the dynamical equations

$$\begin{aligned} \partial_t \tilde{K}_j^i + \tilde{N}^l \partial_l \tilde{K}_j^i + \tilde{K}_l^i \partial_j \tilde{N}^l - \tilde{K}_j^l \partial_l \tilde{N}^i + \tilde{D}^i \tilde{D}_j \tilde{N} \\ - ^{(3)}\tilde{R}_j^i \tilde{N} - \tilde{N} \tilde{K} \tilde{K}_j^i = \frac{\tilde{N}}{2} \left[\left(\tilde{S} - \tilde{E} \right) \delta_j^i - 2\tilde{S}_j^i \right], \end{aligned} \quad (47)$$

where $\tilde{K} \equiv \tilde{K}_i^i$. The trace of this equation yields

$$\partial_t \tilde{K} + \tilde{N}^l \partial_l \tilde{K} + ^{(3)}\tilde{\Delta} \tilde{N} - \tilde{N} \tilde{K}_{ij} \tilde{K}^{ij} = \frac{\tilde{N}}{2} \left(\tilde{S} + \tilde{E} \right), \quad (48)$$

where $^{(3)}\tilde{\Delta} \equiv \tilde{D}^i \tilde{D}_i$.

Further introducing $\tilde{Q}^2 \equiv \tilde{Q}^c \tilde{Q}_c$, one computes

$$\tilde{E}[\tilde{\phi}] = \frac{1}{2} \left(\tilde{\Pi}^2 + \tilde{Q}^2 \right) + U(\tilde{\phi}), \quad (49)$$

$$\tilde{J}[\tilde{\phi}] = -\tilde{\Pi} \tilde{Q}_a, \quad (50)$$

$$\tilde{S}_{ab}[\tilde{\phi}] = \tilde{Q}_a \tilde{Q}_b - \tilde{h}_{ab} \left[\frac{1}{2} \left(\tilde{Q}^2 - \tilde{\Pi}^2 \right) + U(\tilde{\phi}) \right], \quad (51)$$

while

$$\tilde{S}[\tilde{\phi}] = \frac{a}{2} \left(3\tilde{\Pi}^2 - \tilde{Q}^2 \right) - 3U(\tilde{\phi}) \quad (52)$$

and

$$\tilde{S}[\tilde{\phi}] - \tilde{E}[\tilde{\phi}] = \left(\tilde{\Pi}^2 - \tilde{Q}^2 \right) - 4U(\tilde{\phi}). \quad (53)$$

The “total” quantities entering the right hand side of the 3 + 1 field equations are then

$$\tilde{E} = \frac{1}{2} \tilde{Q}^2 + \frac{1}{2} \tilde{\Pi}^2 + U(\tilde{\phi}) + \tilde{E}^{(m)}, \quad (54)$$

$$\tilde{J}_a = -\tilde{\Pi} \tilde{Q}_a + \tilde{J}_a^{(m)}, \quad (55)$$

$$\begin{aligned} \tilde{S}_{ab} = & -\tilde{h}_{ab} \left[\frac{1}{2} \left(\tilde{Q}^2 - \tilde{\Pi}^2 \right) + U(\tilde{\phi}) \right] \\ & + \tilde{Q}_a \tilde{Q}_b + \tilde{S}_{ab}^{(m)}, \end{aligned} \quad (56)$$

while

$$\tilde{S} = -3U(\tilde{\phi}) - \frac{\tilde{Q}^2}{2} - \frac{3\tilde{\Pi}^2}{2} + \tilde{S}^{(m)}, \quad (57)$$

$$\tilde{S} - \tilde{E} =$$

$$\tilde{\Pi}^2 - \tilde{Q}^2 - 4U(\tilde{\phi}) + \tilde{S}^{(m)} - \tilde{E}^{(m)}, \quad (58)$$

$$\tilde{S} + \tilde{E} = 2\tilde{\Pi}^2 - 2U(\tilde{\phi}) + \tilde{S}^{(m)} + \tilde{E}^{(m)}. \quad (59)$$

The Hamiltonian constraint becomes

$$\begin{aligned} ^{(3)}\tilde{R} + \tilde{K}^2 - \tilde{K}_{ij} \tilde{K}^{ij} + \frac{\tilde{\Pi}^2}{2} + \frac{\tilde{Q}^2}{2} \\ = \tilde{E}^{(m)} + U(\tilde{\phi}), \end{aligned} \quad (60)$$

while the momentum constraint (46) is

$$\tilde{D}_l \tilde{K}_i^l - \tilde{D}_i \tilde{K} + \tilde{\Pi} \tilde{Q}_i = \tilde{J}_i^{(m)}, \quad (61)$$

the dynamical equation (47) is written as

$$\begin{aligned} & \partial_t \tilde{K}_j^i + \tilde{N}^l \partial_l \tilde{K}_j^i + \tilde{K}_l^i \partial_j \tilde{N}^l - \tilde{K}_j^l \partial_l \tilde{N}^i + \tilde{D}^i \tilde{D}_j \tilde{N} \\ & - {}^{(3)}\tilde{R}_j^i \tilde{N} - \tilde{N} \tilde{K} \tilde{K}_j^i + \frac{\tilde{N}}{2} 2U(\tilde{\phi}) \delta_j^i + \tilde{N} \tilde{Q}^i \tilde{Q}_j \\ & = \frac{\tilde{N}}{2} \left[\left(\tilde{S}^{(m)} - \tilde{E}^{(m)} \right) \delta_j^i - 2\tilde{S}_j^{(m) i} \right] \end{aligned} \quad (62)$$

with trace

$$\begin{aligned} & \partial_t \tilde{K} + \tilde{N}^l \partial_l \tilde{K} + {}^{(3)}\tilde{\Delta} \tilde{N} - \tilde{N} \tilde{K}_{ij} \tilde{K}^{ij} - \\ & - \tilde{N} \tilde{\Pi}^2 = \frac{\tilde{N}}{2} \left(-2U(\tilde{\phi}) + \tilde{S}^{(m)} + \tilde{E}^{(m)} \right) \end{aligned} \quad (63)$$

where [17]

$$\begin{aligned} & \mathcal{L}_{\tilde{n}} \tilde{\Pi} - \tilde{\Pi} \tilde{K} - \tilde{Q}^c \tilde{D}_c \left(\ln \tilde{N} \right) - \tilde{D}_c \tilde{Q}^c = -\tilde{\Box} \tilde{\phi} \\ & = -\frac{dU}{d\tilde{\phi}}. \end{aligned} \quad (64)$$

In vacuo, the initial data $(\tilde{h}_{ij}, \tilde{K}_{ij}, \tilde{\phi}, \tilde{Q}_i, \tilde{\Pi})$ on an initial hypersurface Σ_0 obey the constraints (60) and (61) plus

$$\tilde{Q}_i - \tilde{D}_i \tilde{\phi} = 0, \quad \tilde{D}_i \tilde{Q}_j = \tilde{D}_j \tilde{Q}_i. \quad (65)$$

In the presence of matter, the variables $\tilde{E}^{(m)}$, $\tilde{J}_a^{(m)}$, and $\tilde{S}_{ab}^{(m)}$ are also assigned on the initial hypersurface. Fixing a gauge corresponds to prescribing lapse and shift. The system (60)-(63) contains only first-order derivatives in both space and time once the d'Alembertian $\tilde{\Box} \tilde{\phi}$ is written in terms of $\tilde{\phi}$, $\tilde{\nabla}^c \tilde{\phi} \tilde{\nabla}_c \tilde{\phi}$, and their derivatives by using eq. (64). From this point on, everything proceeds as in Ref. [17] and the nonminimal coupling factor $f(\phi(\tilde{\phi}))$ in $\tilde{T}_{ab}^{(m)} = T_{ab}^{(m)}/f^2$ does not have consequences because it contains no derivatives of $\tilde{S}_{ab}^{(m)}$, $\tilde{J}_a^{(m)}$, or $\tilde{E}^{(m)}$. The reduction to a first-order system indicates that the Cauchy problem is well-posed in vacuo and well-formulated in the presence of those forms of matter for which it is well-formulated in general relativity. We do not duplicate Salgado's analysis here, and we refer the reader to [17, 20] for details.

Equivalence between conformal frames

At this point, it is clear that the initial value formulation is well-posed in the Einstein frame if it is well-posed in the Jordan frame, and vice-versa. The two frames are equivalent also from the point of view of the Cauchy problem, contrary to folklore and recurring statements in the

literature. To this regard, it is often remarked that the mixing of the spin two and spin zero degrees of freedom g_{ab} and ϕ in the Jordan frame makes these variables an inconvenient set for formulating the initial value problem, which is consequently not well-posed in the Jordan frame, while the Einstein frame variables $(\tilde{g}_{ab}, \tilde{\phi})$ admit a well-posed Cauchy problem completely similar to that of general relativity. (A rather casual remark in the well-known paper [39] (see also the more recent Ref. [23]) seems to have been quite influential in this respect, without further questioning of it in later literature until the recent work of Salgado [17]). In the light of this work, which is carried out completely in the Jordan frame, the standard lore is obviously false. Old works also hinted to the fact that the Cauchy problem is well-posed *in the Jordan frame* for two special scalar-tensor theories: Brans-Dicke theory with a free scalar ϕ [46], and the theory of a scalar field conformally coupled to the Ricci curvature [47]. The implementation, in the Jordan frame, of a full 3+1 formulation à la York [48] for use in numerical applications further dispels the myth that the Cauchy problem is not well-posed in the Jordan frame [20].

Were this folklore true, the Jordan and Einstein frames would be physically inequivalent with regard to the Cauchy problem, but we have shown that this is not the case. In fact, the equivalence between the two conformal frames does not break down even when the scalar field redefinition $\phi \rightarrow \tilde{\phi}$ fails. The Jordan and Einstein frame are still equivalent, with respect to the initial value formulation, for general scalar-tensor theories and, therefore, they are equivalent at the classical level, thus dissipating residual doubts left in this regard in [22]. However, the two conformal frames seem to be inequivalent at the quantum level ([21, 22] and references therein).

V. EXAMPLE: THE NON-MINIMALLY COUPLED SCALAR FIELD

We are finally ready to consider, as an example, the theory of a scalar field coupled nonminimally to the Ricci curvature. In fact this example, many features of which are well-known, has sometimes already guided us through this paper. The action is

$$\begin{aligned} S_{NMC} = \int d^4x \sqrt{-g} \left[\left(\frac{1}{2\kappa} - \frac{\xi \phi^2}{2} \right) R - \frac{1}{2} \nabla^c \phi \nabla_c \phi \right. \\ \left. - V(\phi) + \alpha_m \mathcal{L}^{(m)} \right], \end{aligned} \quad (66)$$

where ξ is a dimensionless coupling constant (in our notations, conformal coupling corresponds to $\xi = 1/6$), and α_m is a suitable coupling constant. The field equations are

$$(1 - \kappa\xi\phi^2) G_{ab} = \kappa \left[\nabla_a \phi \nabla_b \phi - \frac{1}{2} g_{ab} \nabla^c \phi \nabla_c \phi - V(\phi) g_{ab} + \xi (g_{ab} \square - \nabla_a \nabla_b) (\phi^2) + T_{ab}^{(m)} \right], \quad (67)$$

$$\square\phi - \frac{dV}{d\phi} - \xi R\phi = 0 \quad (68)$$

(see [15, 49] for a discussion of alternative ways of writing the field equations). By neglecting the matter part of the action, the Ricci curvature can be eliminated from the Klein-Gordon equation obtaining

$$\frac{1 + (6\xi - 1) \kappa\xi\phi^2}{1 - \kappa\xi\phi^2} \square\phi - \frac{\kappa\xi\phi}{1 - \kappa\xi\phi^2} [(1 - 6\xi) \nabla^c \phi \nabla_c \phi + 4V] - \frac{dV}{d\phi} = 0. \quad (69)$$

Singularities of the first kind correspond to $f(\phi) = \frac{1}{\kappa} - \xi\phi^2 = 0$, or to the critical scalar field values

$$\phi = \pm\phi_* \equiv \frac{\pm 1}{\sqrt{\kappa\xi}} \quad (70)$$

and can only occur if $\xi > 0$. They correspond to diverging effective gravitational coupling

$$G_{eff} = \frac{G}{1 - \kappa\xi\phi^2}, \quad (71)$$

which changes sign if the scalar ϕ crosses $\pm\phi_*$. The requirement $f(\phi) > 0 \forall \phi$ avoids these critical values. However, one could decide to momentarily ignore the physical interpretation of the theory and to allow these critical values from a purely mathematical point of view; then, the latter return to haunt the Cauchy problem and predictability.

The quantity f_1 is, in this theory,

$$f_1(\phi) = \frac{1 + \kappa\xi(6\xi - 1)\phi^2}{1 - \kappa\xi\phi^2}. \quad (72)$$

The roots of the equation $f_1 = 0$, which exist if $0 < \xi < 1/6$, are the critical values of the second kind

$$\pm\phi_c \equiv \frac{\pm 1}{\sqrt{\kappa\xi(1 - 6\xi)}}. \quad (73)$$

The non-uniqueness of the solutions and the breakdown of the Cauchy problem marked by the critical values $\pm\phi_*, \pm\phi_c$ are seen as follows. When $\phi = \phi_0 = \text{const.}$ and matter is absent, the theory reduces to vacuum general relativity with a cosmological constant, and the field equations reduce to

$$G_{ab} + \Lambda g_{ab} = 0, \quad \Lambda = \frac{\kappa V(\phi_0)}{1 + \kappa\xi\phi_0^2}, \quad (74)$$

$$V'_0 + \xi R\phi_0 = 0. \quad (75)$$

The trace of eq. (74) gives $R = 4\Lambda$ which, compared with eq. (75) in turn implies that

$$R = \frac{-V'_0}{\xi\phi_0}. \quad (76)$$

If $\phi = \pm\phi_*$ (the critical values of the first kind), then it must be $V_0 = 0$ and, therefore $R_{ab} = 0$. The Klein-Gordon equation yields the extra necessary condition $V'_0 = 0$. All vacuum solutions of general relativity ($R_{ab} = 0$) are also solutions of the field equations (67) and (68) with $\phi = \pm\phi_*$.

If instead $\phi = \pm\phi_c$ (the second kind of critical values), eqs. (74) and (75) yield

$$\Lambda = \frac{\kappa(1 - 6\xi) V(\pm\phi_c)}{2(1 - 3\xi)}, \quad (77)$$

and

$$V'(\pm\phi_c) = \mp \frac{2\sqrt{\kappa\xi(1 - 6\xi)} V(\pm\phi_c)}{1 - 3\xi}. \quad (78)$$

At these critical scalar field values of the second kind, the dynamical equation (69) for ϕ loses all the second derivatives of ϕ (contained in $\square\phi$) and, consequently, the dynamics for this field (except for special solutions satisfying $\square\phi = 0$). In isotropic FLRW spaces, solutions are known which cross the critical values $\pm\phi_c$, or ϕ is identically equal to one of these values. However, the situation can be worse: there are physical curvature and shear singularities in anisotropic Bianchi models [25, 28, 31, 50]. Moreover, Barcelo and Visser [30] find diverging Ricci scalar R for spherically symmetric wormhole solutions. These examples correspond to solutions which cannot cross the barrier $\phi = \pm\phi_c$.

The conformal transformation to the Einstein frame is $g_{ab} \rightarrow \tilde{g}_{ab} = \Omega^2 g_{ab}$ with

$$\Omega = \sqrt{1 - \kappa\xi\phi^2} \quad (79)$$

and the redefinition bringing the scalar field into canonical form is

$$d\tilde{\phi} = \frac{\sqrt{1 - \kappa\xi(1 - 6\xi)}}{1 - \kappa\xi\phi^2} d\phi. \quad (80)$$

By integrating the last equation, the Einstein frame scalar $\tilde{\phi}$ can be explicitly expressed in terms of ϕ as

$$\tilde{\phi} = \sqrt{\frac{3}{2\kappa}} \ln \left[\frac{\xi\sqrt{6\kappa\phi^2} + \sqrt{1 - \xi(1 - 6\xi)\kappa\phi^2}}{\xi\sqrt{6\kappa\phi^2} - \sqrt{1 - \xi(1 - 6\xi)\kappa\phi^2}} \right] + f(\phi), \quad (81)$$

where

$$f(\phi) = \left(\frac{1-6\xi}{\kappa\xi} \right)^{1/2} \arcsin \left(\sqrt{\xi(1-6\xi)\kappa\phi^2} \right) \quad (82)$$

for $0 < \xi < 1/6$ and

$$f(\phi) = \left(\frac{6\xi-1}{\kappa\xi} \right)^{1/2} \operatorname{arcsinh} \left(\sqrt{\xi(6\xi-1)\kappa\phi^2} \right) \quad (83)$$

for $\xi > 1/6$, while

$$\tilde{\phi} = \sqrt{\frac{3}{2\kappa}} \ln \left(\frac{\sqrt{6/\kappa} + \phi}{\sqrt{6/\kappa} - \phi} \right) \quad \text{if } |\phi| < \sqrt{\frac{6}{\kappa}}, \quad (84)$$

or

$$\tilde{\phi} = \sqrt{\frac{3}{2\kappa}} \ln \left(\frac{\phi - \sqrt{6/\kappa}}{\phi + \sqrt{6/\kappa}} \right) \quad \text{if } |\phi| > \sqrt{\frac{6}{\kappa}} \quad (85)$$

for $\xi = 1/6$.

The Einstein frame action is

$$S = \int d^4x \sqrt{-\tilde{g}} \left\{ \frac{\tilde{R}}{2\kappa} - \frac{1}{2} \tilde{g}^{ab} \tilde{\nabla}_a \tilde{\phi} \tilde{\nabla}_b \tilde{\phi} - U(\tilde{\phi}) + \tilde{\alpha}_m(\phi) \mathcal{L}^{(m)} \right\} \quad (86)$$

where

$$U(\tilde{\phi}) = \frac{V[\phi(\tilde{\phi})]}{\left[1 - \kappa\xi\phi^2(\tilde{\phi}) \right]^2} \quad (87)$$

and

$$\tilde{\alpha}_m(\tilde{\phi}) = \frac{\alpha_m}{\left[1 - \kappa\xi\phi^2(\tilde{\phi}) \right]^2}. \quad (88)$$

When $\phi = \pm\phi_*$, the conformal transformation of the metric breaks down, while the redefinition of the scalar field becomes invalid when $\phi = \pm\phi_c$. In this last situation, one can still use the variables (\tilde{g}_{ab}, ϕ) to define an Einstein frame in which the action is simply

$$S = \int d^4x \sqrt{-\tilde{g}} \left(\frac{\tilde{R}}{2\kappa} - \frac{V(\phi)}{(1 - \kappa\xi\phi^2)^2} + \frac{\alpha_m}{(1 - \kappa\xi\phi^2)^2} \mathcal{L}^{(m)} \right) \quad (89)$$

with no dynamics for ϕ , which becomes an auxiliary field and can be assigned arbitrarily.

VI. TOY MODELS

In this section we consider toy models in the context of point particle dynamics, which help obtaining some insight into the “singularities” of the first and second kind of scalar-tensor theories.

Let us first consider the point particle action

$$S = \int dt L(x(t), \dot{x}(t), y(t), \dot{y}(t)) \\ = \int dt \left[\frac{\dot{x}^2 f(y)}{2} - \frac{w(y) \dot{y}^2}{2} - J(x) \right] \quad (90)$$

where an overdot denotes differentiation with respect to the time t , the generalized coordinates x and y mimic the metric g_{ab} and the scalar ϕ , respectively, the functions $f(y)$ and $w(y)$ represent $f(\phi)$ and $\omega(\phi)$, while J represents the matter sources. Since we are interested in the purely gravitational sector, we will set J to zero in most of the following.

The coordinate x is cyclic and the Euler-Lagrange equations $\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}^i} \right) - \frac{\partial L}{\partial x^i} = 0$ ($i = 1, 2$) yield

$$\dot{x}(y) = C, \quad (91)$$

$$w(y) \ddot{y} + \frac{w'(y) \dot{y}^2}{2} + \frac{f'(y) \dot{x}^2}{2} = 0, \quad (92)$$

where a prime now denotes differentiation with respect to y and C is an arbitrary integration constant.

i) The analogue of a singularity of the first kind $f(\phi) = 0$ in a domain is $f(y) \equiv 0$ on an interval, which implies $C = 0$ and

$$w(y) \ddot{y} + \frac{w'(y) \dot{y}^2}{2} = 0. \quad (93)$$

This equation admits the first integral

$$\int_{y_0}^y dy' \sqrt{|w(y')|} = C_1 (t - t_0), \quad (94)$$

where C_1 and t_0 are integration constants. Let us consider now, for the sake of illustration, the choice $w(y) = y$ yielding the solution

$$y(t) = C_2 (t - t_*)^{2/3}, \quad (95)$$

with C_2 and t_* integration constants. Note that, because $f \equiv 0$, there is no equation for $x(t)$ and the dynamics of this variable are lost: the initial value problem is not well-posed because $x(t)$ can be assigned arbitrarily and is not determined uniquely by initial data (x_0, \dot{x}_0) at an initial time t_0 .

ii) Let us consider now the situation in which $f(y)$ vanishes at isolated points y_* mimicking the critical scalar field values ϕ_* . Then, in the system (91) and (92), either $C = 0$ or else $\dot{x} \rightarrow \infty$ as $y \rightarrow y_*$. If $C \neq 0$, then $\dot{x} = C/f(y) \rightarrow \pm\infty$ as $f(y) \rightarrow 0^\pm$ and, therefore, also $x(t) \rightarrow \pm\infty$ or the solution is not of class \mathcal{C}^1 and its derivative does not exist. In the first case, a barrier separates the regions $f(y) > 0$ and $f(y) < 0$, however special solutions which traverse the barrier $y = y_*$ can in principle exist.

If $C = 0$, an exceptional solution $x(t) = \text{const.}$, $y(t) = C_2(t - t_*)^{2/3}$ passes through this barrier, however this corresponds to the special value $C = 0$ and it disappears when $C \neq 0$.

iii) Let us consider now the case $w(y) \equiv 0$ on an interval, corresponding to a singularity of the second kind $f_1(y) = 0$ on a domain. Then, we are left with

$$\dot{x}f(y) = C, \quad (96)$$

$$\dot{x}f'(y) = 0. \quad (97)$$

From eq. (97), either $x(t) = \text{const.}$ and then it must be $C = 0$ with no equation left to determine $y(t)$, or the equation $f'(y) = 0$ is an algebraic (or transcendental, but not a differential) equation that determines constant values y_* of y (if it admits roots). Assuming that $f(y_*) \neq 0$, then $x_*(t) = \frac{C}{f(y_*)}t + x_0$. The solutions $(x_*(t), y_*(t))$, if they exist, are the only ones and correspond to exceptional initial conditions and, in this sense, there are no dynamics for y .

iv) We can now consider the situation in which $w(y)$ vanishes at isolated points y_c , mimicking isolated singularities of the second kind $f_1(\phi_c) = 0$. Consider, for example, the choice $w(y) = y$, $f(y) = y - 1$, for which the system (91) and (92) reduces to

$$\dot{x}(y - 1) = C, \quad (98)$$

$$y\ddot{y} + \frac{\dot{y}^2}{2} + (y - 1)\frac{\dot{x}^2}{2} = 0. \quad (99)$$

Assuming that y is not identically unity, it is $y\ddot{y} + \frac{\dot{y}^2}{2} + \frac{C^2}{2(y-1)} = 0$; at $y = 0$ one has $\dot{y}_c = \pm C$ and one can not assign arbitrary initial conditions on the “hypersurface” analogue $y = 0$, but only the initial data $(x_0, \dot{x}_0, y_0, \dot{y}_0) = (x_0, -C, 0, \pm C)$ are allowed there, where C and x_0 are arbitrary constants. The region allowed to the dynamics in the four-dimensional space $(x_0, \dot{x}_0, y_0, \dot{y}_0)$ is only two-dimensional, due to the presence of the first integral (91) and of the additional first integral [54]

$$\frac{w(y)\dot{y}^2}{2} - \frac{C^2}{2f(y)} = \mathcal{H} = \text{const.} \quad (100)$$

If a solution attains the critical value $y = 0$, it must assume the values $(x_0, \dot{x}_0, y_0, \dot{y}_0) = (x_0, -C, 0, \pm C)$ there, for which the “energy” \mathcal{H} can only take the values

$$\mathcal{H} = \frac{C^2}{2} [w(0) + 1] \quad (101)$$

(where eq. (91) has been used) everywhere along the orbits of the solutions.

The analogue of the Einstein frame

Let us consider again the toy model action (90); the transformation to the Einstein frame for scalar-tensor gravity is a change of variables modelled by the transformation $(x, y) \rightarrow (\xi, \eta)$ defined by

$$d\xi = \sqrt{f(y)} dx, \quad (102)$$

$$d\eta = \sqrt{w(y)} dy. \quad (103)$$

In terms of these new variables, the action (90) is rewritten in the canonical form

$$S = \int dt \left[\frac{\dot{\xi}^2}{2} - \frac{\dot{\eta}^2}{2} - J(x(\xi, y)) \right], \quad (104)$$

which mimicks the Einstein frame representation of the scalar-tensor action with the matter sources J now depending on both the “new metric” ξ and the “scalar field” y , or η through $y(\eta)$. Zeros of either $f(y)$ or $w(y)$ make the analog of the conformal transformation plus scalar field redefinition (102), (103) ill-defined. Moreover, if $f(y) \neq 0$ and only $w(y)$ vanishes, one can still consider an “Einstein frame” representation with the variables ξ and y , in terms of which the action is simply

$$S = \int dt \left[\frac{\dot{\xi}^2}{2} - J(\xi, y) \right]. \quad (105)$$

It is clear that, similar to the case considered before for scalar-tensor gravity, there are no dynamics for the variable y , which can be assigned arbitrarily [55]. This is bad news if this variable plays a physical role because there are no equations to rule it and it can only be assigned from outside the theory, which is akin to invoking a miracle to produce any effect that one may desire and results in a complete loss of predictive power for the theory.

Singular points of ODEs

To conclude this section, we comment on the fact that, in the theory of ordinary differential equations (ODEs), it is rather common to encounter situations in which the phase space is divided into two disconnected regions, with only exceptional solutions, or a restricted submanifold of solutions, crossing the boundary between these two regions. Consider, for example, the ODE

$$t^2 \ddot{y} - 2y = 0, \quad (106)$$

which has $t = 0$ as a regular singular point. Two linearly independent solutions are

$$y_1(t) = t^2, \quad y_2(t) = \frac{1}{t}. \quad (107)$$

The first solution crosses undisturbed the $t = 0$ “barrier”, while the second cannot (that is, $t = 0$ is a barrier to at least some of the solutions). Consider also the third solution in $(-\infty, 0) \cup (0, +\infty)$

$$y_3(t) = \begin{cases} 0 & \text{if } t \leq 0, \\ t^2 & \text{if } t \geq 0. \end{cases} \quad (108)$$

y_3 is continuous with its first derivative at $t = 0$ (but the second derivative is not defined there). Now, $y_1(t)$ and $y_3(t)$ are linearly independent solutions which satisfy the same initial conditions $(y(0), \dot{y}(0)) = (0, 0)$ at $t = 0$. These two otherwise distinct solutions intersect at the origin of the phase space, which signals the breakdown of the initial value formulation at $t = 0$. It is not surprising, therefore, that for the more complicated systems of partial differential equations ruling scalar-tensor theories, the Cauchy problem breaks down at the analogue of singular points of the equations. Depending on the particular form of the coupling functions $f(\phi)$ and $\omega(\phi)$, special solutions crossing the barrier may or may not exist. The situation in ODE theory in which no such special solution exists is exemplified by the equation

$$t^2 \ddot{y} + 5t \dot{y} + 3y = 0. \quad (109)$$

For $t > 0$ and for $t < 0$, two linearly independent solutions are $y_1(t) = 1/t$ and $y_2(t) = 1/t^3$. No choice of the arbitrary constants $C_{1,2}$ in the general solution

$$y(t) = \frac{C_1}{t} + \frac{C_2}{t^3} \quad (110)$$

in $(-\infty, 0) \cup (0, +\infty)$ produces a solution crossing the barrier $t = 0$.

VII. CONCLUSIONS

In principle, two kinds of “singularities” for the Cauchy problem are possible in general scalar-tensor theories: those (“first kind”) at which $f(\phi) = 0$, and those (“second kind”) at which $f_1(\phi) = 0$. Although statements that these should be rejected outright have been voiced in the literature [23], solutions corresponding to critical values of the BD-like scalar field of both first [24, 27, 30, 37, 50] and second kind [24, 25, 28, 31, 50] have been studied in the literature. Critical points of the second kind may appear benign when studied in a spatially homogeneous and isotropic FLRW universe, but they reveal their true nature of geometrical singularities when analyzed in anisotropic Bianchi models [25, 28, 31, 50]. Here, following recent developments in the theory of the Cauchy problem of scalar-tensor gravity, we have shown that the latter is not well-posed at any of those critical points. The solutions are not unique and

the physics becomes unpredictable. Physically, this is associated to a change in sign of the effective gravitational coupling (19), which diverges at both kinds of critical points. It seems that nature abhors such changes from attractive to repulsive gravity (and vice-versa) which, formally, only take place through a singularity of G_{eff} . This, however, says nothing about exotic forms of matter which can source repulsive gravity through the field equations, a completely different and seemingly perfectly legitimate mechanism from the mathematical point of view (although the violation of all the energy conditions would certainly be questionable on physical grounds).

To conclude, we remark that a possible cure for the problem of Palatini $f(R)$ gravity (already outlined in Refs. [25, 45, 50]) could be the insertion into the gravitational action of terms that introduce higher order derivatives into the field equations. Then, the dropping out of $\square\phi$ from the field equations will be immaterial. However, unless such higher derivative terms appear in the Gauss-Bonnet combination, they will introduce ghost fields. A study of the initial value problem for these Gauss-Bonnet-corrected theories will be presented elsewhere.

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- [51] Strictly speaking, a separate analysis is needed for each different form of matter, but it is expected that “reasonable” forms of matter (perfect fluids, minimally coupled scalar fields, Maxwell field, *etc.*) have a well-posed Cauchy problem, on the basis of the fact that they do in general relativity and that the relevant field equations do not change much in scalar-tensor gravity, once the gravitational sector is proved to be well-behaved with respect to the initial value problem [6, 18].
- [52] In [37], a scenario was proposed which exhibits a singularity-free early universe with a conformally coupled and self-coupled scalar field ϕ asymptotically emerging from a Minkowski space corresponding to the critical values ϕ_* in the past.

- [53] *Cf.* Ref. [44] for conformal continuation past these points.
- [54] Eq. (100) can be easily derived from the field equations by multiplying eq. (92) by \dot{y} and integrating; vice-versa, one verifies that $d\mathcal{H}/dt = 0$ by using the equations of motion.
- [55] This situation should not be confused with the $\omega = 0$ Brans-Dicke equivalent of metric $f(R)$ gravity, for which

there are indeed non-trivial dynamics even if no kinetic term for ϕ appears in the action. In fact, there, a dynamical equation containing $\square\phi$ still exists to rule the evolution of ϕ . It is instead Palatini $f(R)$ gravity which has no dynamical equation for ϕ because $\square\phi$ completely disappears from the relevant equation [5].